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Shocked, Turbulent, Particle-Laden Flow in Explosions and High-Speed Combustors

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14. ABSTRACT
A multi-scale method is developed that couples a macro-scale, high-order resolution particle-mesh method for computation of particle-laden compressible flow in blast waves and high-speed combustors, with a meso-scale, full-resolution, high-fidelity first principles model for direct numerical simulations of shocked flows. At the macro scale the particles are modeled using reduced point cloud methods that rely on semi-empirical forcing models. The semi-empirical models are closed through metamodels that assimilate meso-scale physics through simulations in a multi-dimensional parameter space. The performance of several meta-models are compared and assessed. Meso, macro and multi-scale computations of shock interaction with a cloud of particles are performed for a range of parameters to test the method

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MULTI-SCALE METHOD FOR COMPUTATION OF SHOCKED, TURBULENT, PARTICLE-LADEN FLOW IN EXPLOSIONS AND HIGH-SPEED COMBUSTORS

AFOSR GRANT NO. F9550-12-1-0115

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Objectives

The objective of this project was to develop and test a multi-scale method for simulation of explosions and combustion processes where fluid turbulence and shocks have a strong mutual interaction with solid particulates. We seek to advance the development of particle transport models through an improved multi-scale closure of macro-models using high-resolution micro-scale simulations.

Approach

The multi-scale method couples a macro-scale, high-order resolution particle-mesh method for computation of particle-laden compressible flow models, with a meso-scale, full-resolution, high-fidelity first principles model for direct numerical simulations of shocked flows. At the macro scale the particles are modeled using reduced point cloud methods that rely on semi-empirical forcing models. The semi-empirical models are closed through metamodels that assimilate meso-scale physics through simulations in a multi-dimensional parameter space. The performance of several meta-models are compared and assessed. Meso, macro and multi-scale computations of shock interaction with a cloud of particles are performed for a range of parameters to test the method.

Macro-micro coupling using metamodeling techniques

In a typical multiscale modeling problem, information needs to be transferred across disparate length scales. In the current problem of a shock wave passing through a gas laden with solid particles [**1**] the particle scale (of the order of microns) is governed by meso-scale conservation equations for each of the solid and fluid phases **[1]** separately; on the other hand the system scale (of the order of meters) is governed by macro-scale conservation equations which average over the solid and fluid phases**[2]**. This averaging process results in source terms in the macro-scale governing equations, e.g. particle drag etc. Typically such source terms are obtained from empirical models constructed from physical experiments. Not only are the experiments expensive, but also such experiments can only be performed in a limited

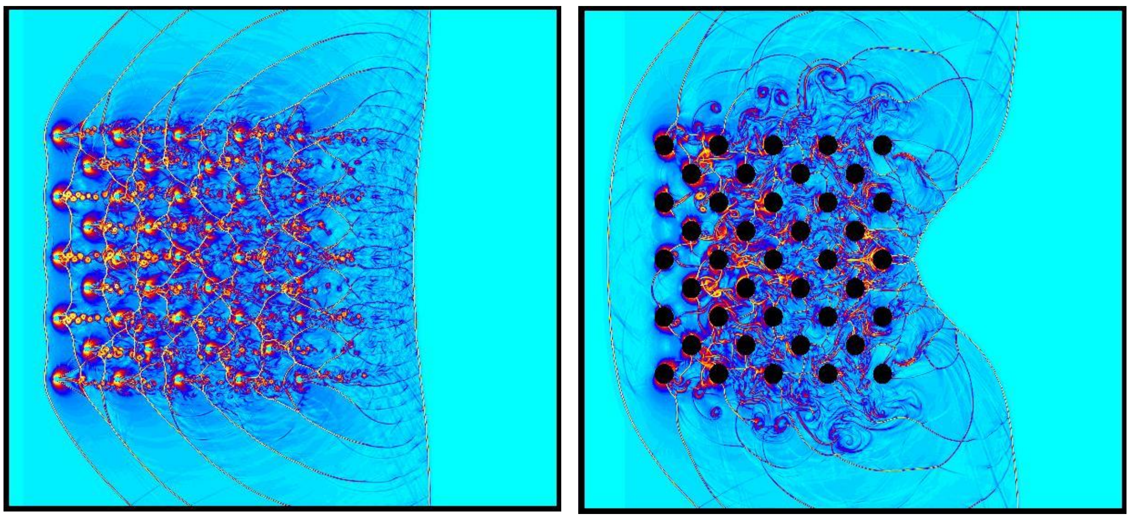

Figure 1. Schlieren images of shock interaction with particle clouds obtained using high resolution meso-scale simulations. Left: Low particle loading; Right: High particle loading

parameter space (e.g. particle volume fraction, shock strength etc), which may be vastly different from the shock strength, volume fraction etc encountered by the particles in the actual macro-scale. The current research has demonstrated the use of high-resolution meso-scale computational experiments (Figure 1) which serve as surrogates to physical experiments in constructing the aforementioned source terms. The novelty of such an approach is that the computational experiments can be designed on a parameter space that is of relevance to the meso-scale. In the current work, a massively parallel computational code, SCIMITAR3D has been used to perform **[1]** the meso-scale computations. The research has demonstrated the efficient use of metamodels to “lift” the relevant information from the mesoscale to the macro-scale equations; the meso-scale simulations provide a numerical drag law which can be readily used as a source term in macro-scale governing equations. Finally, this numerical drag law has been used in an Eulerian-Lagrangian macro-scale code [**2**] to study shock interactions with particle curtains in shock tubes and the results are compared with experimental data in such systems.

Determining a suitable metamodeling technique

The performance of five metamodeling techniques, the Polynomial stochastic collocation (PSC), Adaptive stochastic collocation (ASC), Radial Basis Function Neural Network (RBFANN), Kriging and Dynamic Kriging (DKG) methods, is compared for use as the coupling algorithm or a metamodel in a multi-scale solver. The magnitude and the rates of the representation error of each of these methods has been characterized by their sum-of-squares error in representing various empirical drag manifolds. The convergence results are shown in Figure 2.

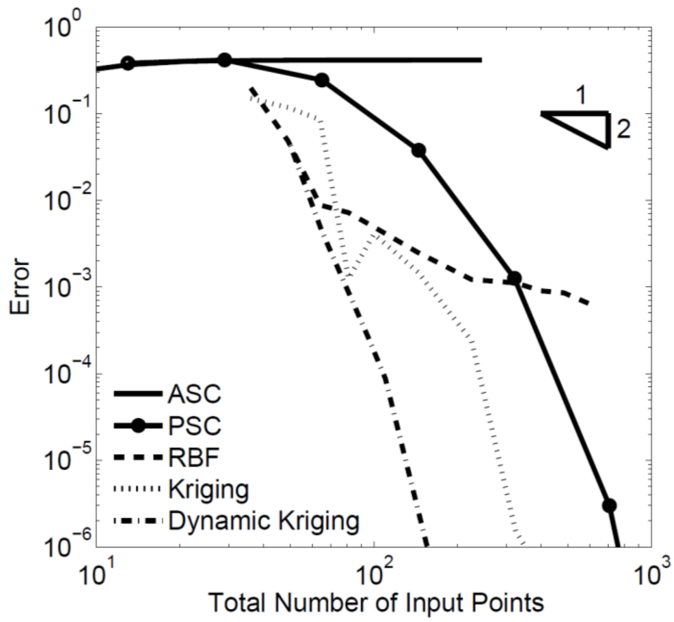

Figure 2. Comparison of the convergence behavior of the five metamodeling approaches tested. The number of inputs (meso-scale simulations) required for constructing the metamodel for an empirical drag manifold is shown to be the least for the Dynamic Kriging Approach.

For a large number of training points, the SC methods generally approximate most of the hypersurfaces most accurately. In particular, the adaptive refinement of the ASC method around steep gradients on the interior of the input domain captures the complex regions of high gradient in the hypersurfaces of the empirical drag functions tested. But the number of input points required to accurately predict a hypersurface using the SC methods is roughly equal to or more than 100 for most of the hypersurfaces. Because in a multiscale modeling framework, input points correspond to high resolution mesoscale computations, generation of such a high number of input points is expensive. Additionally, both the PSC and ASC methods are constructed using a strict predetermined nodal architecture and lack the flexibility of the Kriging and the RBFANN methods with respect to placement of input data. For example, with the SC-based methods, expanding the parameter space would entail discarding the input from a previous set of data or introducing additional interpolation errors. This would result in waste of computational time and resources when an expanded parameter space is required. The input points of the RBFANN and the Kriging methods can be randomly placed throughout the domain with little or no effect on the convergence of the metamodel. Because of this flexibility, the parameter space can be expanded to include a larger domain of approximation while continuing to utilize previous data. However, the RBFANN and Kriging methods have the highest sum-of-squares error in approximating most of the functions tested and do not converge at as high of rates as the SC methods. Additionally, the Kriging method using the DACE code does not converge monotonically in some cases. The parameter estimation technique integrated within the DACE code (i.e. the use of modified Hooke and Jeeves algorithm) leads to the selection of a local extremum value of the shape parameter θ as the global extremum in the maximum likelihood estimation process.

The non-monotonic convergence of the Kriging method is circumvented in the DKG method by a Global Pattern Search (GPS) algorithm using a maximum likelihood estimator with a penalty function and by the use of dynamic selection of correlation models and mean structure. The DKG method is not only monotonically convergent for all the functions considered in the current work, but at roughly 100 input nodes, has either the lowest sum-of-squares error or is close to the lowest (i.e. relative to the SC methods). Therefore, metamodels may be built using less than 100 training points using the DKG method. Thus, for the functions approximated in the current work, the DKG method is the optimal choice to serve as the coupling algorithm for the multi-scale solver.

Macro-scale modeling and testing

To facilitate multi-scale modeling, a macro-scale model is formulated that relies on metamodels. Reduced models are developed for the particle phase based on averaging techniques. Through averaging techniques both Lagrangian and Eulerian formulations are derived for the particle phase. Closure terms that arise through averaging represent particles stresses and cross-correlation of the particle variables with the fluid. Semi-empirical functions that are closed through meta-models force the particle kinematics and dynamics.

Since the meta-model mantles are inquired for every particle and every time step, an algorithmically economic look-up table is created from the Kriging model above on an orthogonal basis. With an increasing order of interpolation, the macro-scale models are shown to converge. Integral to the convergence is the source forcing of the particle phase on the gas conservation equations. The singular source is regularized through a mixed polynomial approximation that preserves the accuracy of the high-order resolution WENO/Spectral based Navier-Stokes solver. Extensive component testing is conducted with the macro-scale algorithm that verify general theorems of hyperbolic systems with singular sources.

Extensive tests have been conducted on a case of particle cloud with varying initial shapes. The resolution and behavior of normal, wake and shear instabilities are investigated. Wake instabilities are strongly dependent on the initial cloud shape and orientation (Fig. 3). Through a linear perturbation analysis, particles are shown to potentially enhance instabilities of shear instabilities in the flow. Macro-scale simulations verify the behavior. In high-speed flows, numerical Carbuncle instabitlites create low velocities that originate in the shock and bleed into the cloud. The multi-scale algorithm is shown to converge with increasing sample rates.

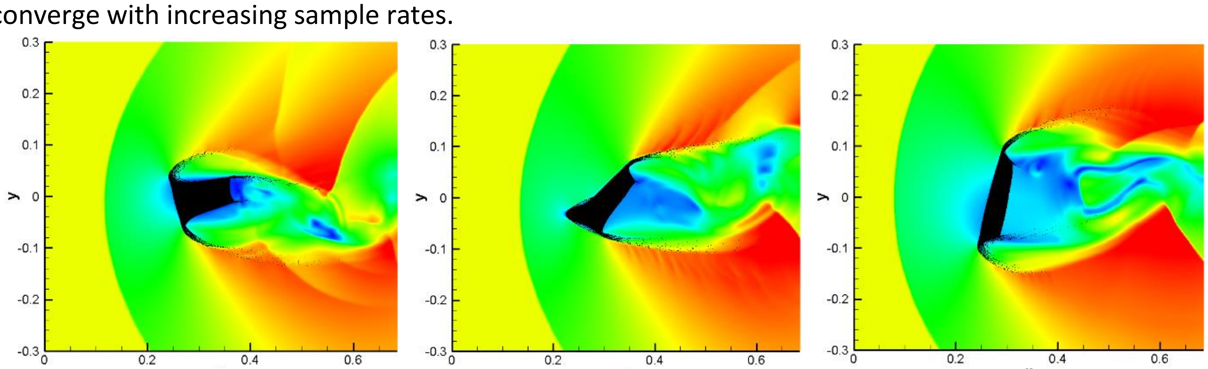

Figure 3. Macro-scale and multi-scale testing of the interaction between a shock and an initially rectangular cloud under an angle of attack of 15, 45 and 75 degrees (left to right).

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Udaykumar, H.S.	Professor, U. of Iowa

Publications resulting from this award

1. Sen, O., Davis, S. Jacobs, G.B , Udaykumar, H.S. Evaulation of Convergence Behavior of Metamodeling Techniques for Bridging Scales in a Multi-Scale Framework", Journal of Computational Physics, 295, pp. 65-86, 2015.
2. Senatore, G. , Davis, S. , Jacobs, G.B., ``The Effect of Particles on the Stability of Shear Layers with Differential Loading" , Physics of Fluids, Physics of Fluids, 27(3), 2015..
3. Suarez, J.P., Jacobs, G.B., Don, W.S., ``Optimal Scaling for a Regularized Dirac Delta Function in the Numerical Solution of Singular Hyperbolic Conservation Laws" , SIAM Journal of Scientific Computing, 36(4), pp. 1839-1849, 2014.
4. Shotorban, B., Jacobs, G.B. , Ortiz, O. , Truong, Q. , ``An Eulerian-Eulerian Approach for Non-isothermal Interaction of Particles with Compressible Flows'', International Journal of Heat and Mass Transfer , 65, 845-854 2013.
5. Davis, S. L. , Dittmann, T.B. , Jacobs, G.B. , Don, W.S., "Disperson of a Cloud of Particles by a Moving Shock: Effects of Shape, Angle of Rotation and Aspect Ratio", Journal of Applied Mechanics and Technical Physics, 54(6), 2013.
6. Kapahi, A., and H.S. Udaykumar, *Dynamics of void collapse in shocked energetic materials: physics of void-void interactions.* Shock Waves, 2013. 23(6): p. 537-558.
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8. Dillard, S., J. Buchholz, S. Vigmostad, H. Kim, and H.S. Udaykumar, *Techniques to derive geometries for image-based Eulerian computations.* Engineering Computations, 2014. 31(3): p. 530-566.
9. Davis, S., Jacobs, G.B., Don, W.S., ``Carbuncles in Higher-Order Resolution Eulerian-Lagrangian Computation of High-Speed, Particle-Laden Flow ", AIAA-2013-2436, 2013.

10. Davis, S., Sen, O., Udaykumar, H.S., Jacobs, G.B., ``Coupling of Micro-Scale and Macro-Scale Eulerian-Lagrangian Models for the Computation of Shocked, Particle-Laden Flows”, IMECE2013-62521, 2013.
11. Truong, Q., Shotorban, B., and Jacobs, G.B., ``Eulerian-Eulerian Description of the Interaction of a Shock with Particles through Godunov's Scheme”, Proceedings of the ASME 2013 Fluids Engineering Division Summer Meeting, FEDSM2013-16567, 2013.

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Abstract

A self-learning, multi-scale method is developed for simulation of flows containing shocks and particles. The innovative computational tool enables the efficient and accurate determination of the unsteady particle/droplet dynamics and flow phenomena occurring in blasts and high-speed combustors and improves upon existing, widely used low-order macro- scale particle-mesh methods which limitations are showing as a result from a low spatial resolution and a limited statistical representation. The method allows for faster analysis and prototyping of the engineering designs and environments in which particles, droplets, shocks and turbulence are of importance.
The method couples a macro-scale, high-order resolution particle-mesh method for computation of particle-laden compressible, with a meso-scale, full-resolution, high-fidelity first principles model for direct numerical simulations of shocked flows. At the macro scale the particles are modeled using reduced point cloud methods that rely on semi-empirical forcing models. The semi-empirical models are closed through metamodels that assimilate meso-scale physics through simulations in a multi-dimensional parameter space. The method hence combines a high-order spatial and statistical resolution ranging from meso-scale to macro-scale particle and flow scales with computational efficiency
The performance of several meta-models are compared and assessed. A dynamic Kriging meta-model was

preferred, because it converges monotonically and require a low number of samples in a multi-dimensional parameter space. Meso-scale simulations demonstrate the use of high-resolution meso-scale computational experiments for the generation of meta-model mantles. Macro-scale models are developed that improve the coupling with the meta-model. The macro-scale is tested for a shock interaction with a cloud of particles for a range of parameters. Multi-scale computations are performed on this case that show the proof-of -concept of the method.

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Archival Publications (published) during reporting period:

1. Sen, O., Davis, S. Jacobs, G.B , Udaykumar, H.S. Evaulation of Convergence Behavior of Metamodeling Techniques for Bridging Scales in a Multi-Scale Framework", Journal of Computational Physics, 295, pp. 65-86, 2015.
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